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NEWS 3	AUG 09	INSPEC enhanced with 1898-1968 archive
NEWS 4	AUG 28	ADISCTI Reloaded and Enhanced
NEWS 5	AUG 30	CA(SM)/CAplus(SM) Austrian patent law changes
NEWS 6	SEP 21	CA/CAplus fields enhanced with simultaneous left and right truncation
NEWS 7	SEP 25	CA(SM)/CAplus(SM) display of CA Lexicon enhanced
NEWS 8	SEP 25	CAS REGISTRY(SM) no longer includes Concord 3D coordinates
NEWS 9	SEP 25	CAS REGISTRY(SM) updated with amino acid codes for pyrrolysine
NEWS 10	SEP 28	CEABA-VTB classification code fields reloaded with new classification scheme
NEWS 11	OCT 19	LOGOFF HOLD duration extended to 120 minutes
NEWS 12	OCT 19	E-mail format enhanced
NEWS 13	OCT 23	Option to turn off MARPAT highlighting enhancements available
NEWS 14	OCT 23	CAS Registry Number crossover limit increased to 300,000 in multiple databases
NEWS 15	OCT 23	The Derwent World Patents Index suite of databases on STN has been enhanced and reloaded
NEWS 16	OCT 30	CHEMLIST enhanced with new search and display field
NEWS 17	NOV 03	JAPIO enhanced with IPC 8 features and functionality
NEWS 18	NOV 10	CA/CAplus F-Term thesaurus enhanced
NEWS 19	NOV 10	STN Express with Discover! free maintenance release Version 8.01c now available
NEWS 20	NOV 20	CAS Registry Number crossover limit increased to 300,000 in additional databases
NEWS 21	NOV 20	CA/CAplus to MARPAT accession number crossover limit increased to 50,000
NEWS 22	DEC 01	CAS REGISTRY updated with new ambiguity codes
NEWS 23	DEC 11	CAS REGISTRY chemical nomenclature enhanced
NEWS 24	DEC 14	WPIDS/WPINDEX/WPIX manual codes updated
NEWS 25	DEC 14	GBFULL and FRFULL enhanced with IPC 8 features and functionality
NEWS 26	DEC 18	CA/CAplus pre-1967 chemical substance index entries enhanced with preparation role
NEWS 27	DEC 18	CA/CAplus patent kind codes updated
NEWS 28	DEC 18	MARPAT to CA/CAplus accession number crossover limit increased to 50,000
NEWS 29	DEC 18	MEDLINE updated in preparation for 2007 reload
NEWS 30	DEC 27	CA/CAplus enhanced with more pre-1907 records

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DICTIONARY FILE UPDATES: 7 JAN 2007 HIGHEST RN 916885-50-2

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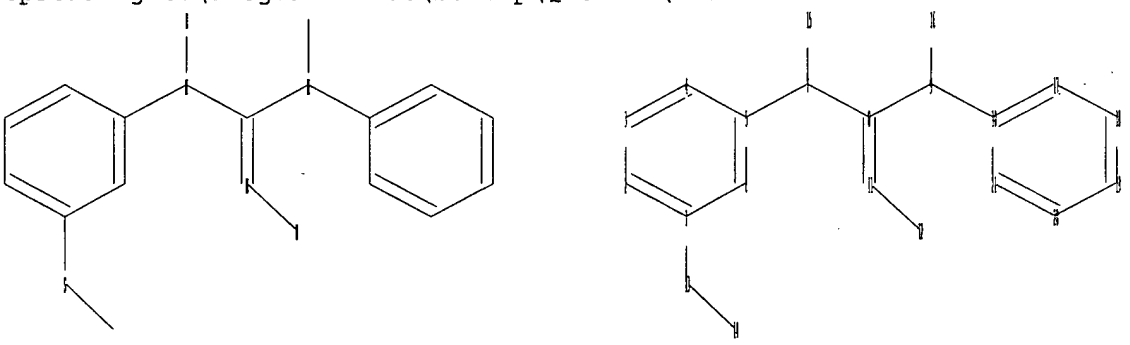

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ring nodes :
1  2  3  4  5  6  10  17  18  19  20  21
chain bonds :
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ring bonds :
1-2  1-6  2-3  3-4  4-5  5-6  10-17  10-21  17-18  18-19  19-20  20-21
exact/norm bonds :
1-13  5-7  7-8  8-9  8-11  9-10  9-16  13-14
exact bonds :
7-15  11-12
normalized bonds :
1-2  1-6  2-3  3-4  4-5  5-6  10-17  10-21  17-18  18-19  19-20  20-21


Match level :
1:CLASS  2:CLASS  3:CLASS  4:CLASS  5:CLASS  6:CLASS  7:Atom  8:Atom  9:Atom
10:CLASS  11:Atom  12:Atom  13:Atom  14:Atom  15:Atom  16:Atom  17:CLASS  18:CLASS
19:CLASS  20:CLASS  21:CLASS



L1      STRUCTURE UPLOADED

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L2   QUE L1

=> d L1
L1 HAS NO ANSWERS
L1                STR
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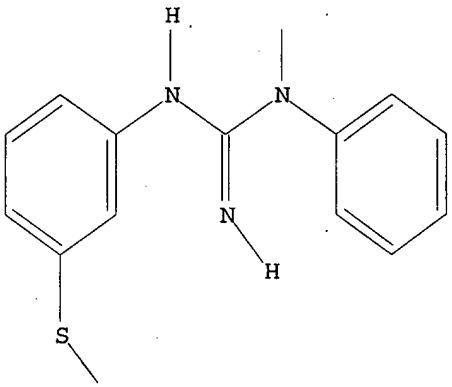


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Structure attributes must be viewed using STN Express query preparation.


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FULL SEARCH INITIATED 09:09:13 FILE 'REGISTRY'
FULL SCREEN SEARCH COMPLETED -      499 TO ITERATE

100.0% PROCESSED      499 ITERATIONS                              78 ANSWERS
SEARCH TIME: 00.00.01

L3           78 SEA SSS FUL L1

=> file caplus
COST IN U.S. DOLLARS                          SINCE FILE      TOTAL
                                                   ENTRY    SESSION
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FILE 'CAPLUS' ENTERED AT 09:09:20 ON 08 JAN 2007
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FILE COVERS 1907 - 8 Jan 2007 VOL 146 ISS 3
FILE LAST UPDATED: 7 Jan 2007 (20070107/ED)

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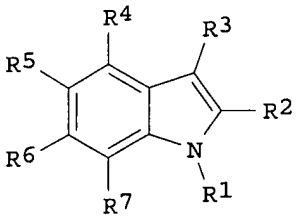
=> s L3
L4 24 L3

=> d L4 1-24 bib abs

L4 ANSWER 1 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:1204362 CAPLUS
DN 145:505331
TI Substituted indole compounds having NOS inhibitory activity and their preparation and pharmaceutical composition
IN Maddaford, Shawn; Ramnauth, Jailall; Rakhit, Suman; Patman, Joanne; Renton, Paul; Annedi, Subhash C.
PA Can.
SO U.S. Pat. Appl. Publ., 129pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 2006258721	A1	20061116	US 2006-404267	20060413
PRAI US 2005-670856P	P	20050413		

GI



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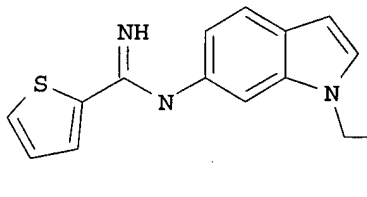


II

AB The invention features compds. of formula I as inhibitors of nitric oxide synthase (NOS), particularly those that selectively inhibit neuronal nitric oxide synthase (nNOS) in preference to other NOS isoforms. The NOS

inhibitors of the invention, alone or in combination with other pharmaceutically active agents, can be used for treating or preventing conditions such as, for example, stroke, reperfusion injury, neurodegeneration, head trauma, CABG, migraine headache with and without aura, migraine with allodynia, central post-stroke pain (CPSP), neuropathic pain, morphine/opioid induced tolerance and hyperalgesia. Compds. of formula I wherein R1 is H, (un)substituted C1-6 alkyl, (un)substituted C1-4 alkylaryl, and (un)substituted C1-4 alkylheterocyclyl; R2 and R3 are independently H, halo, (un)substituted C1-6 alkyl, (un)substituted C6-10 aryl, (un)substituted C1-4 alkylaryl, (un)substituted C2-9 bridge heterocyclyl, etc.; R4 and R7 are independently H, F, C1-6 alkyl, and C1-6 alkoxy; R5 is H, R5AC(NH)NH(CH2)r, and R5ANHC(S)NH(CH2)r; r is an integer from 0 to 2; R5A is (un)substituted C1-6 alkyl, (un)substituted C6-10 aryl; (un)substituted C1-4 alkylaryl, etc.; R6 is H, R6AC(NH)(CH2)r and R6ANHC(S)(CH2)r; R6A is equal to R5A; and their pharmaceutically acceptable salts and prodrugs thereof are claimed. Example compound II was prepared by N-alkylation of 6-nitroindole with N,N-dimethyl-2-chloroethylamine; the resulting N-(2-dimethylaminoethyl)-6-nitroindole underwent reduction to give the corresponding 6-aminoindole derivative, which underwent addition to thiophene-2-carboximidothionic acid Ph ester hydrobromide to give compound II. All the invention compds. were evaluated for their NOS inhibitory activity. From the assay, it was determined that compound II exhibited IC50 values of 8.8 μM against Rat nNOS, 109 μM against Murine iNOS, 211 μM against Bovine eNOS, 1.2 μM against Human nNOS, 60 μM against Human iNOS and 15 μM against Human eNOS.

L4 ANSWER 2 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2006:303970 CAPLUS
DN 145:505191
TI Synthesis and characterization of N-[2-chloro-5-(methylthio)phenyl]-N'-[3-(methylthio)phenyl]-N'-[11C]methylguanidine [11C]CNS 5161, a candidate PET tracer for functional imaging of NMDA receptors
AU Zhao, Yongjun; Robins, Edward; Turton, David; Brady, Frank; Luthra, Sajinder K.; Arstad, Erik
CS Hammersmith Imanet, London, W12 0NN, UK
SO Journal of Labelled Compounds and Radiopharmaceuticals (2006), 49(2), 163-170
CODEN: JLCRD4; ISSN: 0362-4803
PB John Wiley & Sons Ltd.
DT Journal
LA English
AB N-Methyl-D-aspartate (NMDA) receptors play a key role in excitatory neurotransmission and are linked to a variety of acute and chronic neurodegenerative diseases including epilepsy, schizophrenia, Parkinson disease, and drug abuse. N-[2-Chloro-5-(methylthio)phenyl]-N'-[3-(methylthio)phenyl]-N'-methylguanidine (CNS 5161) is a high affinity ligand (Ki = 1.87 nM) for the NMDA PCP site, which potentially can be used for functional imaging of this receptor. Herein, we report the synthesis of the corresponding positron emission tomog. (PET) tracer [11C]CNS 5161 by [11C]methylation of the desmethyl guanidine precursor. [11C]CNS 5161 was synthesized with a decay corrected radiochem. yield of 10% within 45 min after end of bombardment (EOB). The final product was prepared in a sterile saline solution suitable for clin. studies with a radiochem. purity of >96% and a specific activity of 41 GBq/mmol at time of injection.
RE.CNT 19 THERE ARE 19 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 3 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:1059129 CAPLUS
DN 142:32998
TI Compositions of a cyclooxygenase-2 selective inhibitor and a cannabinoid agent for the treatment of central nervous system damage
IN Stephenson, Diane T.; Taylor, Duncan P.
PA Pharmacia Corporation, USA

SO PCT Int. Appl., 177 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2004105699	A2	20041209	WO 2004-US16496	20040526
WO 2004105699	A3	20051215		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
US 2006160776	A1	20060720	US 2004-854586	20040526
PRAI US 2003-473820P	P	20030528		

OS MARPAT 142:32998
AB The present invention provides compns. and methods for the treatment of central nervous system damage in a subject. More particularly, the invention provides a combination therapy for the treatment of a central nervous system ischemic condition or a central nervous system traumatic injury comprising the administration to a subject of a cannabinoid agent in combination with a cyclooxygenase-2 selective inhibitor.

L4 ANSWER 4 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:814610 CAPLUS
DN 142:459221
TI In vivo evaluation of [11C]N-(2-chloro-5-thiomethylphenyl)-N'-(3-methoxy-phenyl)-N'-methylguanidine ([11C]GMOM) as a potential PET radiotracer for the PCP/NMDA receptor
AU Waterhouse, Rikki N.; Slifstein, Mark; Dumont, Filip; Zhao, Jun; Chang, Raymond C.; Sudo, Yasuhiko; Sultana, Abida; Balter, Andrew; Laruelle, Marc
CS Department of Psychiatry, New York State Psychiatric Institute, Columbia University College of Physicians and Surgeons, New York, NY, 10032, USA
SO Nuclear Medicine and Biology (2004), 31(7), 939-948
CODEN: NMBIEO; ISSN: 0969-8051
PB Elsevier Inc.
DT Journal
LA English
AB The development of imaging methods to measure changes in NMDA ion channel activation would provide a powerful means to probe the mechanisms of drugs and device-based treatments (e.g., ECT) thought to alter glutamate neurotransmission. To provide a potential NMDA/PCP receptor PET tracer, we synthesized the radioligand [11C]GMOM (ki = 5.2 ±0.3 nM; log P = 2.34) and evaluated this ligand in vivo in awake male rats and isoflurane anesthetized baboons. In rats, the regional brain uptake of [11C]GMOM ranged from 0.75±0.13% ID/g in the medulla and pons to 1.15±0.17% ID/g in the occipital cortex. MK801 (1 mg/kg i.v.) significantly reduced (24-28%) [11C]GMOM uptake in all regions. D-Serine (10 mg/kg i.v.) increased [11C]GMOM %ID/g values in all regions (10-24%) reaching significance in the frontal cortex and cerebellum only. The NR2B ligand RO 25-6981 (10 mg/kg i.v.) reduced [11C]GMOM uptake significantly (24-38%) in all regions except for the cerebellum and striatum. Blood activity was 0.11±0.03 %ID/g in the controls group and did not vary significantly across groups. PET imaging in isoflurane-anesthetized baboons with high specific activity [11C]GMOM provided fairly uniform regional brain distribution volume (VT) values (12.8-17.1 mL g-1). MK801 (0.5 mg/kg, i.v., n = 1, and 1.0 mg/kg, i.v., n = 1) did not significantly alter regional VT values, indicating a lack of saturable binding. However, the potential

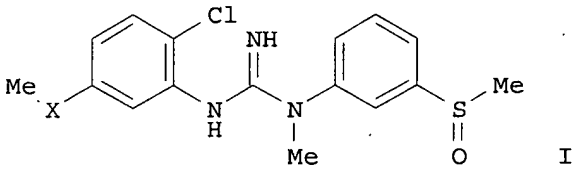
confounding effects associated with ketamine induction of anesthesia along with isoflurane maintenance must be considered because both agents are known to reduce NMDA ion channel activation. Future and carefully designed studies, presumably utilizing an optimized NMDA/PCP site tracer, will be carried out to further explore these hypotheses. We conclude that, even though [11C]GMOM is not an optimized PCP site radiotracer, its binding is altered in vivo in awake rats as expected by modulation of NMDA ion channel activity by MK801, D-serine or RO 25-6981. The development of higher affinity NMDA/PCP site radioligands is in progress.

RE.CNT 49 THERE ARE 49 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:645804 CAPLUS
DN 141:174086
TI Pharmaceutically active compounds containing a guanidine moiety for treatment of neurol. injury and neurodegenerative disorders
IN Durant, Graham J.; Perlman, Michael; Fischer, James B.; Padmanabhan, Seetharamaiyer
PA Cambridge Neuroscience, Inc., USA
SO U.S., 15 pp., Cont.-in-part of U.S. Provisional Ser. No. 63,469.
CODEN: USXXAM
DT Patent
LA English
FAN.CNT 2

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI US 6774263	B1	20040810	US 1998-169028	19981009
PRAI US 1997-63469P	P	19971010		

GI



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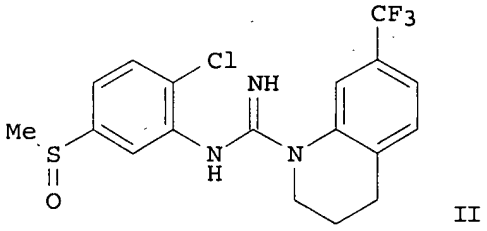

II

AB Compds., such as I (X = S, O) and II, and pharmaceutically acceptable salts thereof, containing a guanidine moiety were prepared for therapeutic use in pharmaceutical compns. for the treatment or prophylaxis of neurol. injury and neurodegenerative disorders. The prepared compds. were assayed for neurol. activity using a rat rotarod motor coordination test.

RE.CNT 14 THERE ARE 14 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 6 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:353140 CAPLUS
DN 140:380634
TI Compositions of cyclooxygenase-2 selective inhibitors and NMDA receptor antagonists for the treatment or prevention of neuropathic pain

IN Cheung, Raymond Y.
PA Pharmacia Corporation, USA
SO U.S. Pat. Appl. Publ., 51 pp.
CODEN: USXXCO
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	US 2004082543	A1	20040429	US 2002-282660	20021029
	WO 2004039371	A2	20040513	WO 2003-US33089	20031017
	WO 2004039371	A3	20040617		
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	AU 2003277440	A1	20040525	AU 2003-277440	20031017
PRAI	US 2002-282660	A	20021029		
	WO 2003-US33089	W	20031017		

OS MARPAT 140:380634
AB The present invention provides compns. and methods to treat or prevent neuropathic pain in a subject using a combination of a COX-2 selective inhibitor and a NMDA receptor antagonist.

L4 ANSWER 7 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2004:60459 CAPLUS
DN 140:111134
TI Preparation of phenylguanidine isotopomers for therapeutic use as in vivo diagnosis or imaging of NMDA-mediated disease
IN Brady, Frank; Luthra, Sajinder Kaur
PA Hammersmith Imanet Ltd., UK
SO PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004007440	A1	20040122	WO 2003-GB3078	20030716
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	AU 2003254460	A1	20040202	AU 2003-254460	20030716
	EP 1521741	A1	20050413	EP 2003-764018	20030716
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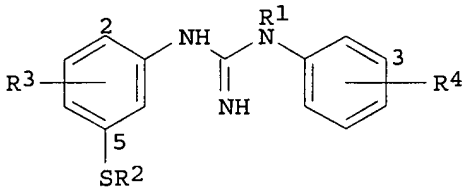
	JP 2005533097	T	20051104	JP 2004-520892	20030716
	US 2005260125	A1	20051124	US 2005-522204	20050118
PRAI	GB 2002-16621	A	20020717		
	WO 2003-GB3078	W	20030716		

OS MARPAT 140:111134
GI



I

AB This invention relates to the preparation of guanidine isotopomers, such as I [R1 = 11CH2R5, (CH2)n18F; R2 = H, C1-4-alkyl; R3 = halogen; R4 = halogen, C1-4-alkyl, C1-4-alkylthio; R5 = H, C1-4-alkyl], for use in diagnosis and tomog. imaging of NMDA-mediated nervous system disease in vivo. Thus, I (R1 = 11CH3, R2 = Me, R2 = 2-Cl, R4 = 3-MeS) was prepared N-alkylation of the corresponding guanidine I (R1 = H, R2 = Me, R2 = 2-Cl, R4 = 3-MeS) with [11C]iodomethane using NaH in MeCN. The prepared guanidines were assayed in rats for biodistribution in body tissue, for radioactivity in blood and plasma, and for NMDA receptor affinity.
RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2003:242167 CAPLUS
DN 138:248536
TI Methods using cholinesterase inhibitors for treating and preventing migraine
IN Pratt, Raymond
PA Eisai Co., Ltd., Japan
SO PCT Int. Appl., 30 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI WO 2003024456	A1	20030327	WO 2002-US29734	20020920
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, OM, PH, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW				
RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
PRAI US 2001-323310P	P	20010920		
US 2002-349244P	P	20020118		

OS MARPAT 138:248536
AB The invention provides safe and effective methods for treating and preventing migraine by administering an effective amount of one or more cholinesterase inhibitors and, optionally, one or more migraine drugs. The invention also provides compns., combinations, and kits comprising one or more cholinesterase inhibitors and one or more migraine drugs. In one embodiment, the cholinesterase inhibitor is donepezil or ARICEPT.
RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:903496 CAPLUS
DN 138:299872
TI Synthesis of [11C] N-(2-chloro-5-thiomethylphenyl)-N'-(3-methoxyphenyl)-N'-

methylguanidine ([11C]GMOM): a candidate PET tracer for imaging the PCP site of the NMDA ion channel
AU Waterhouse, Rikki N.; Dumont, Filip; Sultana, Abida; Simpson, Norman; Laruelle, Marc
CS Department of Psychiatry, Columbia University College of Physicians and Surgeons and New York State Psychiatric Institute, New York, NY, 10032, USA
SO Journal of Labelled Compounds & Radiopharmaceuticals (2002), 45(11), 955-964
CODEN: JLCRD4; ISSN: 0362-4803
PB John Wiley & Sons Ltd.
DT Journal
LA English
AB The N-methyl-D-aspartate (NMDA) ion channel plays an important role in a number of neurodegenerative disorders including stroke, Parkinson's disease, Huntington's Chorea, Alzheimer's disease, schizophrenia and epilepsy. To provide effective radioligands for imaging the PCP binding site of the NMDA ion channel, we synthesized and characterized in vitro the candidate PCP site ligand N-(2-chloro-5-thiomethylphenyl)-N'-(3-methoxyphenyl)-N'-methylguanidine (GMOM: Ki = 5.2 ± 0.3 nM, log P = 2.34). The corresponding PET radiotracer [11C]GMOM was synthesized with a radiochem. yield of 8.4 ± 3.2% EOS and with a specific activity of 1.23 ± 0.25 Ci/μmol EOS (n = 5). The average time required for synthesis, purification and formulation was 52 ± 5 min. The final product was prepared in a sterile saline solution suitable for in vivo use.
RE.CNT 28 THERE ARE 28 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:407966 CAPLUS
DN 138:49371
TI Synthesis and in vitro evaluation of N,N'-diphenyl and N-naphthyl-N'-phenylguanidines as N-methyl-d-aspartate receptor ion-channel ligands
AU Dumont, Filip; Sultana, Abida; Waterhouse, Rikki N.
CS Division of Functional Brain Mapping, Columbia University, New York, NY, 10032, USA
SO Bioorganic & Medicinal Chemistry Letters (2002), 12(12), 1583-1586
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 138:49371
AB A series of N,N'-diphenyl and N-naphthyl-N'-Ph guanidine derivs. was synthesized as potential N-methyl-D-aspartate (NMDA) receptor positron emission tomog. (PET) ligands. The affinity of the different compds. was determined using in vitro receptor binding assays, and their log P values were estimated using HPLC anal. The effect of N'-3 and N'-3,5 substitution on affinity and lipophilicity was examined The Ki values ranged from 1.87 to 839 nM, while log P values between 1.22 and 2.88 were observed
RE.CNT 33 THERE ARE 33 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:370623 CAPLUS
DN 137:232425
TI Synthesis of N-(2-chloro-5-methylthiophenyl)-N'-(3-methyl-thiophenyl)-N'-[3H3]methylguanidine, {[3H3]CNS-5161}
AU Gibbs, Andrew R.; Morimoto, Hiromi; VanBrocklin, Henry F.; Williams, Philip G.; Biegon, Anat
CS Department of Functional Imaging, Lawrence Berkeley National Laboratory, Berkeley, CA, 94720, USA
SO Journal of Labelled Compounds & Radiopharmaceuticals (2002), 45(5), 395-400

CODEN: JLCRD4; ISSN: 0362-4803
PB John Wiley & Sons Ltd.
DT Journal
LA English
OS CASREACT 137:232425
AB The preparation of the title compound, [3H3]CNS-5161, was accomplished in three steps starting with the production of [3H3]iodomethane (CT3I). The intermediate N-[3H3]methyl-3-(thiomethylphenyl)cyanamide was prepared in 77% yield by the addition of CT3I to 3-(thiomethylphenyl)cyanamide, previously treated with sodium hydride. Reaction of this tritiated intermediate with 2-chloro-5-thiomethylaniline hydrochloride formed the guanidine compound [3H3]CNS-5161. Purification by HPLC gave the desired labeled product in an overall yield of 9% with >96% radiochem. purity and a final specific activity of 66 Ci mmol-1.
RE.CNT 16 THERE ARE 16 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 12 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2002:274772 CAPLUS
DN 136:363750
TI Early clinical experience with the novel NMDA receptor antagonist CNS 5161
AU Walters, M. R.; Bradford, A. P. J.; Fischer, J.; Lees, K. R.
CS Western Infirmary, University Department of Medicine and Therapeutics, Glasgow, G11 6NT, UK
SO British Journal of Clinical Pharmacology (2002), 53(3), 305-311
CODEN: BCPHBM; ISSN: 0306-5251
PB Blackwell Publishing Ltd.
DT Journal
LA English
AB Aim was to investigate the safety, tolerability and pharmacokinetics of the novel NMDA antagonist CNS 5161 in humans. Excessive activation of glutamate receptors, especially of the N-methyl-D-aspartate (NMDA) subtype has been associated with neuropathic pain, and brain damage caused by focal ischemia in mature brain or hypoxia-ischemia (HI) in neonates. CNS 5161 is a novel NMDA ion-channel antagonist that interacts with the NMDA receptor/ion channel site to produce a noncompetitive blockade of the actions of glutamate. Pre-clin. studies have demonstrated neuroprotective effects of CNS 5161 in the adult rat model of focal cerebral ischemia, as well as anticonvulsant and analgesic effects. This study reports the first administration of CNS 5161 to man. Its objectives were to investigate the hemodynamic effects of the compound, to assess its safety and tolerability in healthy male volunteers, and to provide some preliminary human pharmacokinetic data. We performed a randomized, double-blind placebo controlled phase 1 dose escalation study of CNS 5161. Volunteers were randomized to receive CNS 5161 or placebo in a ratio of 3:1. Twenty-four of 32 healthy volunteers received i.v. infusion of CNS 5161 over 15 min, followed by serial measurements of plasma drug concentration and hemodynamic observations over 24 h. A dose escalation design was adopted and the volunteers were stratified into eight dosage groups, ranging from 30 μg to 2000 μg. The drug was well tolerated by recipients. Side-effects were dose-related, self limiting and comprised minor subjective sensory symptoms. A dose dependent rise in systolic, mean arterial and diastolic blood pressure was seen in subsequent dosage groups, reaching 23/19 mmHg. Maximal effects were seen between 60 and 120 min after commencement of infusion. All subjects returned to baseline hemodynamic values within 24 h. Putative neuroprotective concns. of CNS 5161 were achieved transiently, although these levels were not sustained. The pharmacokinetic data were best described by a two compartment model. The mean half-life was 2.95 h (s.d. 0.75). Mean clearance was 106 1 h-1 (s.d. 17.8) mean volume of distribution was 296 1 (s.d. 69). These parameters were not significantly affected by body weight This study suggests that CNS 5161 is well tolerated in healthy volunteers within the dose range studied. In addition, information concerning the pharmacokinetics of the compound has been acquired. Studies to investigate the efficacy of the compound in man may now be justified.

RE.CNT 7 THERE ARE 7 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:208093 CAPLUS
DN 134:242673
TI Transdermal administration of n-(2,5-disubstituted phenyl)-n'-(3-substituted phenyl)-n'-methyl guanidines
IN Van Osdol, William W.; Gale, Robert M.; Brandwein, David H.; Padmanabhan, Rama; Sunram, Joan
PA Alza Corporation, USA
SO PCT Int. Appl., 39 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2001019352	A1	20010322	WO 2000-US24682	20000908
	W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, BZ, CA, CH, CN, CR, CU, CZ, DE, DK, DM, DZ, EE, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, TZ, UA, UG, UZ, VN, YU, ZA, ZW				
	RW: GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2384986	A1	20010322	CA 2000-2384986	20000908
	EP 1216036	A1	20020626	EP 2000-964953	20000908
	EP 1216036	B1	20051116		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL				
	AT 309791	T	20051215	AT 2000-964953	20000908
	ES 2249296	T3	20060401	ES 2000-964953	20000908
	US 2003198662	A1	20031023	US 2003-412104	20030411
	US 2004258742	A1	20041223	US 2004-895788	20040720
PRAI	US 1999-153996P	P	19990915		
	US 2000-658649	B1	20000908		
	WO 2000-US24682	W	20000908		
	US 2003-412104	B1	20030411		

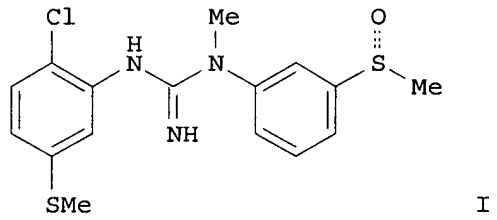
AB A composition for transdermal administration comprises (1) 1-30% a N-(2,5-disubstituted phenyl)-N'-(3-substituted phenyl)-N'-Me guanidine, (2) 0-50% a permeation enhancer, and (3) 30-90% a polymeric carrier. Drug delivery devices and methods for the transdermal administration of a guanidine for the prevention of neuropathic pain, neuropsychol. deficits resulting from cardiac surgery (CABG), and other neurol. disorders are also described. For example, transdermal delivery systems containing 6% guanidine derivative CNS 5161 or its HCl salt CNS 5161A were prepared without or with a permeation enhancer (3% glyceryl monolaurate or 12% lauryl pyroglutamate), and NS 87-2287 acrylate adhesive. Systems with formulations containing the drug as a base displayed higher flux than those with the HCl salt. In addition, systems with formulations containing lauryl pyroglutamate consistently exhibited higher drug flux than formulations with glyceryl monolaurate for formulations with either the drug base or salt.

RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

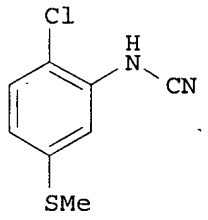
L4 ANSWER 14 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2001:177402 CAPLUS
DN 135:443
TI Identification and characterization of a potential ischemia-selective N-methyl-d-aspartate (NMDA) receptor ion-channel blocker, CNS 5788

AU Padmanabhan, S.; Perlman, M. E.; Zhang, L.; Moore, D.; Zhou, D.; Fischer, J. B.; Durant, G. J.; McBurney, R. N.
CS Cambridge NeuroScience, Inc., Norwood, MA, 02602, USA
SO Bioorganic & Medicinal Chemistry Letters (2001), 11(4), 501-504
CODEN: BMCLE8; ISSN: 0960-894X
PB Elsevier Science Ltd.
DT Journal
LA English
AB The identification and characterization of a potentially ischemia-selective and orally-active sulfoxide based NMDA ion-channel blocker showing good neuroprotective activity, (R)-(+)-N-(2-chloro-5-methylthiophenyl)-N'-(3-methylsulfinylphenyl)-N'-methylguanidine (CNS 5788), is described. Synthesis and in vitro and in vivo studies led to the characterization of a potential ischemia-selective and neuroprotective sulfoxide based ion-channel blocker 10. The R enantiomer has been identified to be orally active and neuroprotective with min. side effects.
RE.CNT 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

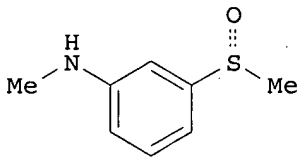
L4 ANSWER 15 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:845048 CAPLUS
DN 134:100623
TI Asymmetric synthesis of a neuroprotective and orally active N-methyl-D-aspartate receptor ion-channel blocker.
AU Padmanabhan, Seetharamaiyer; Lavin, Ruth C.; Durant, Graham J.
CS Cambridge NeuroScience, Inc., Cambridge, MA, 02139, USA
SO Tetrahedron: Asymmetry (2000), 11(17), 3455-3457
CODEN: TASYE3; ISSN: 0957-4166
PB Elsevier Science Ltd.
DT Journal
LA English
OS CASREACT 134:100623
GI



I



II



III

AB Asym. synthesis of N-(2-chloro-5-methylthiophenyl)-N'-(3-methylsulfinylphenyl)-N'-methyl-guanidine (I) was achieved in high enantiomeric excess by condensation of cyanamide II and benzeneamine III. The key step involved asym. oxidation of N-methyl-3-methylthioaniline using (1R)-8,8-Dichloro-10-camphorsulfonyloxaziridine (Davis reagent).
RE.CNT 5 THERE ARE 5 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 16 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 2000:545075 CAPLUS

DN 134:402
TI Neuroprotective, anesthetic, and cardiovascular effects of the NMDA antagonist, CNS 5161A, in isoflurane-anesthetized lambs
AU Bokesch, Paula M.; Kapural, Miranda; Drummond-Webb, Jonathan; Baird, Kevin; Kapural, Leo; Mee, Roger B. B.; Trapp, Bruce; Starr, Norman J.
CS Department of Cardiothoracic Anesthesia, Center for Congenital Heart Disease and Surgery, Cleveland, OH, USA
SO Anesthesiology (2000), 93(1), 202-208
CODEN: ANESAV; ISSN: 0003-3022
PB Lippincott Williams & Wilkins
DT Journal
LA English
AB N-methyl-D-aspartate (NMDA) receptor antagonists are neuroprotective in animal models of cerebral ischemia, but adverse cardiovascular and neurobehavioral effects have precluded their clin. use. The authors present the neuroprotective, anesthetic, and cardiovascular effects of a novel NMDA antagonist, CNS 5161A. Lambs, 4.0-6.5 kg, were anesthetized with isoflurane, intubated, and ventilated and had thermodilution catheters placed in the pulmonary artery and 20-g catheters placed in the femoral artery. The min. alveolar concentration (MAC) of isoflurane was determined using the "bracketing technique.". CNS 5161A was given as a bolus and then as an infusion at three doses. Cardiovascular measurements were determined every 15 min. Other lambs (n = 25) were subjected to cardiopulmonary bypass (CPB) with hypothermic circulatory arrest (HCA) for 120 min. Eighteen received CNS 5161A, and seven received saline vehicle. One hour after CPB, brains were perfusion-fixed and removed for in situ hybridization and immunohistochem. anal. in half of the animals. The other half survived 48 h before their brains were examined for neuronal degeneration. Isoflurane at MAC significantly decreased blood pressure, heart rate, cardiac output, and systemic vascular resistance by 30-48% (n = 16;P < 0.05). CNS 5161A (n = 12) had no significant cardiovascular effects. All concns. of CNS 5161A caused a significant reduction (21-29%) of the MAC of isoflurane (n = 12;P < 0.05). CNS 5161A, at serum concns. greater than 25 ng/mL, completely inhibited c-fos mRNA and c-FOS protein expression in hippocampal neurons after 120 min of HCA, attenuated neuronal degeneration, and improved functional outcome by 47% (P < 0.05). CNS 5161A at neuroprotective concns. before CPB-HCA significantly reduces the MAC of isoflurane without cardiovascular effects.
RE.CNT 37 THERE ARE 37 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 17 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:321805 CAPLUS
DN 131:80
TI CNS-5161 Cambridge NeuroScience Inc
AU Linders, Joannes T. M.
CS Scientific Development Group NV Organon, Oss, 5340 BH, Neth.
SO Current Opinion in Central & Peripheral Nervous System Investigational Drugs (1999), 1(1), 167-170
CODEN: COCDFA; ISSN: 1464-844X
PB Current Drugs Ltd.
DT Journal; General Review
LA English
AB A review with 25 refs. Cambridge NeuroScience is developing CNS-5161, an N-methyl-D-aspartate (NMDA) ion channel blocker, as a potential treatment for neuropathic pain and migraine. It is in phase I development for migraine and neuropathy. Boehringer Ingelheim has the right to negotiate a development and marketing agreement for CNS-5161 for the treatment of neurol. deficits from cardiac surgery [203771], but is not developing the product [231830].
RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 18 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1999:265890 CAPLUS
DN 130:281875
TI Preparation of N-[(methylsulfinyl)phenyl]guanidines as neuroprotectants
IN Durant, Graham J.; Perlman, Michael; Fischer, James B.; Padmanabhan, Seetharamaiyer
PA Cambridge Neuroscience, Inc., USA
SO PCT Int. Appl., 37 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9918962	A1	19990422	WO 1998-US21395	19981009
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, GW, ML, MR, NE, SN, TD, TG				
	CA 2306276	A1	19990422	CA 1998-2306276	19981009
	AU 9910767	A	19990503	AU 1999-10767	19981009
	EP 1041986	A1	20001011	EP 1998-953372	19981009
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO				
	JP 2001519393	T	20011023	JP 2000-515597	19981009
PRAI	US 1997-63469P	P	19971010		
	WO 1998-US21395	W	19981009		

AB Title compds., e.g., MeSZNHC(:NH)NMeC6H4(SOMe)-3.HCl (I) (Z = 2-chloro-1,5-phenylene), were prepared Thus, 3-(MeS)C6H4NHMe was oxidized and the product hydrochloride condensed with 2-chloro-5-methylthiophenylcyanamide to give I.
RE.CNT 1 THERE ARE 1 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 19 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1999:64675 CAPLUS
DN 130:148681
TI Combination antiinfective drug therapies comprising aminoglycoside antibiotics and N,N'-disubstituted guanidines
IN Gwynne, David I.; Durant, Graham J.
PA Cambridge Neuroscience, Inc., USA
SO PCT Int. Appl., 130 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9902145	A1	19990121	WO 1998-US13640	19980706
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, GM, GW, HR, HU, ID, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
	RW: GH, GM, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, CY, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	AU 9882784	A	19990208	AU 1998-82784	19980706
PRAI	US 1997-51860P	P	19970707		
	WO 1998-US13640	W	19980706		

OS MARPAT 130:148681
AB Methods and compns. are provided for treatment of infections, including

Gram-neg. and Gram-pos. bacterial infections, comprising administering an aminoglycoside antibiotic in combination with a substituted guanidine or other compound as disclosed. Preferred methods and compns. of the invention will be effective against infections previously treated with aminoglycoside antibiotics, but with decreased occurrence of ototoxicity.

RE.CNT 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 20 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1998:119668 CAPLUS
DN 128:316907
TI Synthesis and Pharmacological Evaluation of N-(2,5-Disubstituted phenyl)-N'-(3-substituted phenyl)-N'-methylguanidines As N-Methyl-D-aspartate Receptor Ion-Channel Blockers. [Erratum to document cited in CA128:212660]
AU Hu, Lain-Yen; Guo, Junqing; Magar, Sharad S.; Fischer, James B.; Burke-Howie, Kathleen J.; Durant, Graham J.
CS Cambridge NeuroSci., Inc., Cambridge, MA, 02139, USA
SO Journal of Medicinal Chemistry (1998), 41(6), 1006
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB The generic structure for Table 4 has been corrected

L4 ANSWER 21 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1998:94768 CAPLUS
DN 128:176172
TI Methods of treatment of eye trauma and disorders with substituted guanidines and other compounds
IN McBurney, Robert N.
PA Cambridge Neuroscience, Inc., USA; McBurney, Robert N.
SO PCT Int. Appl., 92 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9804131	A1	19980205	WO 1997-US13203	19970725
	W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE, DK, EE, ES, FI, GB, GE, GH, HU, IL, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ, PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG, US, UZ, VN, YU, ZW				
	RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	US 6242198	B1	20010605	US 1996-686494	19960725
	CA 2261765	A1	19980205	CA 1997-2261765	19970725
	AU 9739654	A	19980220	AU 1997-39654	19970725
	AU 742404	B2	20020103		
	EP 918460	A1	19990602	EP 1997-937042	19970725
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, FI				
	JP 2000515895	T	20001128	JP 1998-509048	19970725
	KR 2000029518	A	20000525	KR 1999-700559	19990123
	US 6358696	B1	20020319	US 2000-635309	20000809
	US 2003027801	A1	20030206	US 2002-60101	20020129
	US 6673557	B2	20040106		
PRAI	US 1996-686494	A2	19960725		
	WO 1997-US13203	W	19970725		
	US 2000-635309	A3	20000809		

OS MARPAT 128:176172
AB Methods using substituted guanidines and other compds. are provided for

treatment of eye disorders and injury, including methods for treatment of reduced flow of blood or other nutrients to retinal tissue and/or optic nerve, methods for treatment of retinal ischemia and trauma, and methods for treatment for optic nerve injury/damage.

RE.CNT 3 THERE ARE 3 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 22 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1998:35396 CAPLUS
DN 128:212660
TI Synthesis and pharmacological evaluation of N-(2,5-disubstituted phenyl)-N'-(3-substituted phenyl)-N'-methylguanidines as N-methyl-D-aspartate receptor ion-channel blockers
AU Hu, Lain-Yen; Guyo, Junqing; Magar, Sharad S.; Fischer, James B.; Burke-Howie, Kathleen J.; Durant, Graham J.
CS Cambridge NeuroSci., Inc., Cambridge, MA, 02139, USA
SO Journal of Medicinal Chemistry (1997), 40(26), 4281-4289
CODEN: JMCMAR; ISSN: 0022-2623
PB American Chemical Society
DT Journal
LA English
AB In the mammalian central nervous system, the N-methyl-D-aspartate (NMDA) subclass of glutamate receptors may play an important role in brain diseases such as stroke, brain or spinal cord trauma, epilepsy, and certain neurodegenerative diseases. Compds. which specifically antagonize the actions of the neurotransmitter glutamate at the NMDA receptor ion-channel site offer a novel approach to treating these disorders. Cerestat (aptiganel, CNS 1102) is currently undergoing clin. trial for the treatment of traumatic brain injury and stroke. Previously, the authors reported that analogs of N-1-naphthyl-N'-(3-ethylphenyl)-N'-methylguanidine bound to the NMDA receptor ion-channel site with high potency and selectivity. Recently, mols. active at both σ receptors and NMDA receptor sites were investigated. A series of substituted diphenylguanidines which are structurally related to N-1-naphthyl-N'-(3-ethylphenyl)-N'-methylguanidine was prepared Compds. containing appropriate substitution pattern in one of the Ph rings of diphenylguanidines displayed high affinity. N-(2,5-dibromophenyl)-N'-(3-ethylphenyl)-N'-methylguanidine (I) had potency at both σ receptors and NMDA receptor sites; I also showed high efficacy in vivo in a neonatal rat excitotoxicity model. Further studies indicated that substituent effects were important in this compound series, and 2,5-disubstituted-Ph was the preferred substitution pattern for high-affinity binding at NMDA receptor sites. N-(2-Bromo-5(methylthio)phenyl)-N'-(3-ethylphenyl)-N'-methylguanidine was highly active at NMDA receptor sites. The binding affinity of some guanidines was further enhanced with the appropriate substitution. Two compds. bound to NMDA receptor sites with high potency and selectivity (Ki vs [3H]MK-801: 1.87 and 1.65 nM, resp.,); these compds. are active in vivo in various animal models of neuroprotection. The structure-activity relationships for these compds. at the NMDA receptor ion-channel site are discussed.

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 23 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN
AN 1995:758935 CAPLUS
DN 123:132889
TI Substituted guanidines as NMDA antagonists in treatment of neurological conditions
IN Durant, Graham J.; Hu, Lain-Yen; Magar, Sharad
PA Cambridge Neuroscience, Inc., USA
SO PCT Int. Appl., 38 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9514461	A1	19950601	WO 1994-US13245	19941122
	W: AM, AT, AU, BB, BG, BR, BY, CA, CH, CN, CZ, DE, DK, EE, ES, FI, GB, GE, HU, JP, KE, KG, KP, KR, KZ, LK, LR, LT, LU, LV, MD, MG, MN, MW, NL, NO, NZ, PL, PT, RO, RU, SD, SE, SI, SK, TJ, TT, UA, US, UZ				
	RW: KE, MW, SD, SZ, AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2177081	A1	19950601	CA 1994-2177081	19941122
	AU 9512900	A	19950613	AU 1995-12900	19941122
	AU 705487	B2	19990520		
	EP 739200	A1	19961030	EP 1995-904077	19941122
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	JP 09505591	T	19970603	JP 1995-515132	19941122
	ZA 9409294	A	19951011	ZA 1994-9294	19941123
	US 5922772	A	19990713	US 1995-458809	19950602
	US 5955507	A	19990921	US 1995-459975	19950602
	US 6013675	A	20000111	US 1995-459974	19950602
PRAI	US 1993-156773	A	19931123		
	WO 1994-US13245	W	19941122		

OS MARPAT 123:132889

AB Substituted guanidines RR1NC(:NH)NR2R3 [I; R, R1, R2 = H, (substituted) alkyl, alkenyl, alkynyl, alkoxy, thioalkyl, aminoalkyl, aryl, aralkyl; R3 = (substituted) aryl, thioalkyl, alkylsulfinyl, alkylsulfonyl, haloalkoxy] and pharmaceutically acceptable salts thereof, are effective for treating disorders involving excessive excitation of nerve cells by NMDA receptor agonists. PCP radioligand-binding assays and σ-receptor binding assays were performed with 9 compds., e.g. I (R = 1-naphthyl, R1 = H, R2 = Me, R3 = 3-SMe-C6H4).

L4 ANSWER 24 OF 24 CAPLUS COPYRIGHT 2007 ACS on STN

AN 1995:339509 CAPLUS

DN 122:96529

TI Substituted guanidines for treatment of central nervous system disease

IN Durant, Graham J.; Magar, Sharad; Hu, Lain-Yen

PA Cambridge Neuroscience, Inc., USA

SO PCT Int. Appl., 103 pp.
CODEN: PIXXD2

DT Patent

LA English

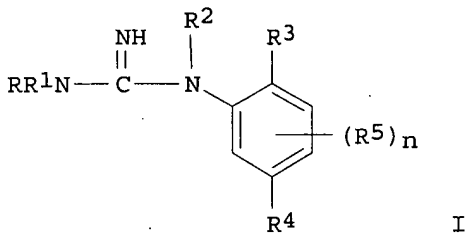
FAN.CNT 2

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 9427591	A1	19941208	WO 1994-US6008	19940527
	W: AU, BB, BG, BR, CA, CZ, FI, HU, JP, KP, KR, LK, LV, MG, MN, MW, NO, NZ, PL, RO, RU, SD, SK, TJ, UA, US				
	RW: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA, GN, ML, MR, NE, SN, TD, TG				
	CA 2163361	A1	19941208	CA 1994-2163361	19940527
	AU 9470473	A	19941220	AU 1994-70473	19940527
	AU 695337	B2	19980813		
	ZA 9403744	A	19950426	ZA 1994-3744	19940527
	EP 705100	A1	19960410	EP 1994-919275	19940527
	EP 705100	B1	20030730		
	R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IE, IT, LI, LU, MC, NL, PT, SE				
	CN 1126434	A	19960710	CN 1994-192610	19940527
	JP 08510754	T	19961112	JP 1995-500988	19940527
	JP 3610368	B2	20050112		
	AT 245977	T	20030815	AT 1994-919275	19940527
	PT 705100	T	20031231	PT 1994-919275	19940527
	ES 2204920	T3	20040501	ES 1994-919275	19940527
	US 6147063	A	20001114	US 1995-458741	19950602
	US 6153604	A	20001128	US 1995-458803	19950602

	US 6156741	A	20001205	US 1995-458506	19950602
	JP 2004285073	A	20041014	JP 2004-140658	20040511
PRAI	US 1993-68522	A	19930527		
	US 1993-156773	B2	19931123		
	JP 1995-500988	A3	19940527		
	WO 1994-US6008	W	19940527		

OS MARPAT 122:96529

GI



I

AB Treatment of the CNS diseases, which involve excitation of nerve cells by agonists of NMDA receptors, comprises administration of substituted guanidines (I; R = R1 = R2 = H, alkyl, alkenyl, alkynyl, alkoxy, alkylthio, aryl, ets; R3 = R4 = R5 = halogen, OH, azido, alkyl, alkenyl, alkynyl, alkoxy, alkylthio, aryl, etc.; n = 0-3) or their salts. The ED80 and the percentage maximum protection against damage to the CNS for some of the I compds. are presented.

```
=> s L4 and labelling
          1165 LABELLING
            16 LABELLINGS
          1179 LABELLING
                 (LABELLING OR LABELLINGS)
L5           0 L4 AND LABELLING

=> s radiolabel
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           278 RADIOLABELS
L6        3901 RADIOLABEL
                 (RADIOLABEL OR RADIOLABELS)

=> s L4 and L6
L7           0 L4 AND L6

=> s imaging compounds
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           105 IMAGINGS
        188383 IMAGING
                 (IMAGING OR IMAGINGS)
        854769 COMPOUNDS
             4 COMPOUNDSES
        854772 COMPOUNDS
                 (COMPOUNDS OR COMPOUNDSES)
       1715845 COMPDS
       2160307 COMPOUNDS
                 (COMPOUNDS OR COMPDS)
L8          24 IMAGING COMPOUNDS
                 (IMAGING(W)COMPOUNDS)

=> s L4 and L8
L9           0 L4 AND L8
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         26883 CARBONS
       1257045 CARBON
                 (CARBON OR CARBONS)
        106338 ISOTOPES
L10       2885 CARBON ISOTOPES
                 (CARBON(W)ISOTOPES)

=> s L4 and L10
L11          0 L4 AND L10

=> s radiolabelled compounds
           267 RADIOLABELLED
        854769 COMPOUNDS
             4 COMPOUNDSES
        854772 COMPOUNDS
                 (COMPOUNDS OR COMPOUNDSES)
       1715845 COMPDS
       2160307 COMPOUNDS
                 (COMPOUNDS OR COMPDS)
L12          6 RADIOLABELLED COMPOUNDS
                 (RADIOLABELLED(W)COMPOUNDS)

=> s L4 and L12
L13          0 L4 AND L12

=> s labelled compounds
          2605 LABELLED
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             4 COMPOUNDSES
        854772 COMPOUNDS
                 (COMPOUNDS OR COMPOUNDSES)
       1715845 COMPDS
       2160307 COMPOUNDS
                 (COMPOUNDS OR COMPDS)
L14         76 LABELLED COMPOUNDS
                 (LABELLED(W)COMPOUNDS)

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         32882 GUANIDINE
          3008 GUANIDINES
L15      33795 GUANIDINE
                 (GUANIDINE OR GUANIDINES)

=> s L14 and L15
L16          0 L14 AND L15

=> s L14 and L4
L17          0 L14 AND L4

=> s radiopharmaceuticals
L18       5137 RADIOPHARMACEUTICALS

=> s L18 and L4
L19          1 L18 AND L4

=> d L19 bib abs

L19  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2004:60459  CAPLUS
DN   140:111134
TI   Preparation of phenylguanidine isotopomers for therapeutic use as in vivo
     diagnosis or imaging of NMDA-mediated disease
```

IN Brady, Frank; Luthra, Sajinder Kaur
PA Hammersmith Imanet Ltd., UK
SO PCT Int. Appl., 23 pp.
CODEN: PIXXD2
DT Patent
LA English
FAN.CNT 1

	PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
PI	WO 2004007440	A1	20040122	WO 2003-GB3078	20030716
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	EP 1521741	A1	20050413	EP 2003-764018	20030716
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	JP 2005533097	T	20051104	JP 2004-520892	20030716
	US 2005260125	A1	20051124	US 2005-522204	20050118
PRAI	GB 2002-16621	A	20020717		
	WO 2003-GB3078	W	20030716		

OS MARPAT 140:111134
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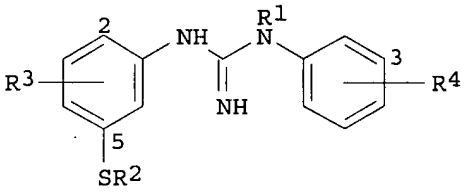

I

AB This invention relates to the preparation of guanidine isotopomers, such as I [R1 = 11CH2R5, (CH2)n18F; R2 = H, C1-4-alkyl; R3 = halogen; R4 = halogen, C1-4-alkyl, C1-4-alkylthio; R5 = H, C1-4-alkyl], for use in diagnosis and tomog. imaging of NMDA-mediated nervous system disease in vivo. Thus, I (R1 = 11CH3, R2 = Me, R2 = 2-Cl, R4 = 3-MeS) was prepared N-alkylation of the corresponding guanidine I (R1 = H, R2 = Me, R2 = 2-Cl, R4 = 3-MeS) with [11C]iodomethane using NaH in MeCN. The prepared guanidines were assayed in rats for biodistribution in body tissue, for radioactivity in blood and plasma, and for NMDA receptor affinity.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

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           79 PHENYLGUANIDINES
L20       670 PHENYLGUANIDINE
              (PHENYLGUANIDINE OR PHENYLGUANIDINES)

=> s isotopomers
L21      5515 ISOTOPOMERS
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=> s L4 and L21
L22           1 L4 AND L21

=> d L22 bib abs

L22  ANSWER 1 OF 1  CAPLUS  COPYRIGHT 2007 ACS on STN
AN   2004:60459  CAPLUS
DN   140:111134
TI   Preparation of phenylguanidine isotopomers for therapeutic use
     as in vivo diagnosis or imaging of NMDA-mediated disease
IN   Brady, Frank; Luthra, Sajinder Kaur
PA   Hammersmith Imanet Ltd., UK
SO   PCT Int. Appl., 23 pp.
     CODEN: PIXXD2
DT   Patent
LA   English
FAN.CNT 1
     PATENT NO.          KIND   DATE        APPLICATION NO.        DATE
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PI   WO 2004007440        A1    20040122    WO 2003-GB3078         20030716
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             GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR,
             LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NI, NO, NZ, OM,
             PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SY, TJ, TM, TN,
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             FI, FR, GB, GR, HU, IE, IT, LU, MC, NL, PT, RO, SE, SI, SK, TR,
             BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG
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     EP 1521741            A1    20050413    EP 2003-764018         20030716
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             IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK
     JP 2005533097         T     20051104    JP 2004-520892         20030716
     US 2005260125         A1    20051124    US 2005-522204         20050118
PRAI GB 2002-16621         A     20020717
     WO 2003-GB3078        W     20030716
OS   MARPAT 140:111134
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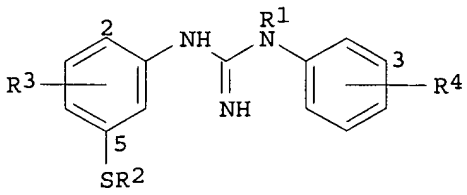

I

AB This invention relates to the preparation of guanidine isotopomers, such as I [R1 = 11CH2R5, (CH2)n18F; R2 = H, C1-4-alkyl; R3 = halogen; R4 = halogen, C1-4-alkyl, C1-4-alkylthio; R5 = H, C1-4-alkyl], for use in diagnosis and tomog. imaging of NMDA-mediated nervous system disease in vivo. Thus, I (R1 = 11CH3, R2 = Me, R2 = 2-Cl, R4 = 3-MeS) was prepared N-alkylation of the corresponding guanidine I (R1 = H, R2 = Me, R2 = 2-Cl, R4 = 3-MeS) with [11C]iodomethane using NaH in MeCN. The prepared guanidines were assayed in rats for biodistribution in body tissue, for radioactivity in blood and plasma, and for NMDA receptor affinity.

RE.CNT 4 THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

```
=> s NMDA compounds
          26917 NMDA
              2 NMDAS
          26917 NMDA
                    (NMDA OR NMDAS)
         854769 COMPOUNDS
              4 COMPOUNDSES
         854772 COMPOUNDS
                    (COMPOUNDS OR COMPOUNDSES)
        1715845 COMPDS
        2160307 COMPOUNDS
                    (COMPOUNDS OR COMPDS)
L23           0 NMDA COMPOUNDS
                    (NMDA(W)COMPOUNDS)

=>

---Logging off of STN---


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FULL ESTIMATED COST                                  109.50     281.81

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